

Observations on Gaussian Bases for Schrödinger's Equation

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Abstract

One of the few methods for generating efficient function spaces for multi-D Schrödinger eigenproblems is given by Garashchuk and Light in *J.Chem.Phys.* 114 (2001) 3929. Their Gaussian basis functions are wider and sparser in high potential regions, and narrower and denser in low ones. We suggest a modification of their approach based on the following observation: In very steep potential regions, wide, sparse, Gaussians should be avoided even if their centers have high potential values. Our numerical results illustrate that a dramatic improvement in accuracy may be obtained in this way. We also compare the errors of collocation to those of a Galerkin approach, test a criterion for scaling Gaussian widths based on deviation from orthogonality of collocation eigenfunctions, and suggest a criterion for scaling Gaussian widths based on Hamiltonian trace minimization.

1 Introduction

Numerical prediction of the properties and behaviour of quantum mechanical systems is a long standing challenge. A major difficulty stems from the high dimensions of such systems. An $n \geq 3$ particle mechanical system generally has $3n - 6$ degrees of freedom, and so to calculate the state of an $n \geq 3$ particle quantum system we must solve a PDE in $3n - 6$ variables. Presently, the limit is $n = 5$ particles (*i.e.* 9 variables) in the largest systems for which many eigenvalues/eigenstates were obtained from Schrödinger's equation [1]. However, there are many larger systems for which numerical predictions would be very useful for chemistry, biology (where many important molecules have more than five

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atoms), and for the emerging field of nano engineering. Clearly, we would like to push the limit further.

To efficiently treat multi-D (*i.e.* multi variable) PDEs we must consider the function spaces where approximations are constructed. Naively, we can form such function spaces by taking tensor products of 1-D function spaces. Many of the 1-D spaces standardly used (*e.g.* Fourier spaces, spaces of orthogonal polynomials of different kinds) have a basis of localized functions peaked above the nodes of a 1-D quadrature formula, these are called 1-D DVRs [2], [3]. The corresponding multi-D DVR basis of the product space consists of localized multi variable functions peaked above the points of \mathcal{G} , the (hyper) rectangular array of nodes of the associated product cubature formula. Typically, at least 10 1-D DVR basis functions are taken for each variable, so the dimension of the product space is at least 10^{3n-6} . This gets much too large, even when the number of particles n is not too big.

DVR bases can give us some insight regarding the inefficiency of multi-D tensor product spaces. Bound solutions of Schrödinger's eigenproblem decay exponentially in high potential regions. Thus, for a given system we can apriori estimate Ω , the region where wavefunctions up to a given energy (eigenvalue) are supported. Typically, Ω is non rectangular and covering it with the rectangular grid \mathcal{G} is inefficient. Many nodes will be outside Ω and therefore many of the multi-D product DVR basis functions will contribute little to the approximation of our wavefunctions. Evidently, efficient localized basis functions should be peaked in Ω , and not outside it. Several approaches have been suggested for obtaining such basis functions.

One very useful solution is to prune a product DVR basis by discarding functions whose nodes lie in high potential regions [3]. Another approach, still in its initial stages, is to construct DVRs based on non product cubatures with various non rectangular node distributions [4]. In both cases the resulting DVR basis functions are orthogonal. However, in these approaches it is not easy to refine the node distribution *within* Ω according to predictable wavefunction properties. Generally, wavefunctions are more oscillatory in low potential regions compared to high ones and node densities in Ω should vary accordingly. Therefore we may try to construct function spaces by appropriately distributing nodes and then placing a localized basis function above each. Gaussians [5] [6] [7], B-splines [8], and inverse multi quadrics [11], have been used in this way. Although the resulting basis functions are not orthogonal, the flexible choice of nodes and basis function shape parameters can give highly accurate results. This has been illustrated in 1-D problems [5] [6]. However the only general method we are aware of for constructing multi-D bases of localized functions whose node density varies with potential values is given by Garashchuk and Light [7].

Here we closely examine the method of [7] for choosing nodes and widths of Gaussian basis func-

tions. Their basis functions are narrow and close together in low potential regions, while they are wide and sparsely distributed in high potential regions. We believe that this needs to be refined in steep potential regions, where points with low and high potential values are very close together. This situation is common in molecular potential surfaces for small nuclear separation. We suggest a simple modification of the nodes/widths choice of [7]. Its essence is to avoid overly wide and sparse basis functions in hard potential regions. We illustrate that this can give a dramatic improvement in accuracy by calculating the eigenfunctions and eigenvalues of two 1-D Morse Hamiltonians. Our results indicate that the algorithm of [7] should be adapted along these lines in the multi-D case.

Our work also explores the use of collocation with Gaussian basis functions. Using collocation, rather than the standard Galerkin approach, is very appealing since calculating integrals of potential matrix elements is avoided. Yang and Peet have previously used collocation with Gaussian basis functions [13], and in their calculations performance was similar to the Galerkin approach. They have used the same basis functions with both methods. However in our calculations basis function widths were adjusted optimally for each method and Galerkin accuracy was much better than collocation. Collocation has many advantages and it can give high quality results as shown in the work of Yang and Peet [13], [14], [15], and in many papers based on it. However, our results illustrate that caution should be exercised before embracing collocation as equally accurate to Galerkin.

Other aspects we examine are the use of collocation with the quasi randomly distributed Gaussians of [7], and using the deviation from orthogonality of eigenfunctions calculated by collocation to guide us in the choice of basis function widths.

The content of this paper follows. In section 2 we describe the distributed Gaussian bases used for Schrodinger's equation leading up to [7], then we overview the collocation approach. In section 3 we discuss the nodes/widths choice of [7], suggest improvements, and raise a few further questions about collocation and Gaussian basis functions. Section 4 gives numerical results for two 1-D Morse Hamiltonians. Finally, we conclude and suggest some future directions in section 5.

2 Distributed Gaussian bases and collocation

Here we discuss the application of distributed Gaussian bases and collocation in the Schrödinger eigenproblem, *i.e.* the problem of finding eigenvalues and eigenfunctions of the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(x) . \quad (1)$$

We concentrate on the problem of finding all bound states below an energy cutoff E_{max} , *i.e.* all eigenfunctions $\{\psi_n\}$ and eigenvalues $\{E_n\}$ belonging to the discrete part of the spectrum with $E_n \leq E_{max}$.

Several researchers have studied the use of Gaussian basis functions for this problem¹. We pick up an important thread in this research by considering the work of Hamilton and Light [5], and continuing to Poirier and Light [6], and to Garashchuk and Light [7].

The basis functions used in [5] are real Gaussians

$$\varphi_i(x) = \eta_i e^{-cw_i(x-x_i)^2} \quad i = 1, \dots, n \quad (2)$$

whose parameters are named as follows.

- x_i is called the center or node of φ_i .
- $w_i > 0$ is the width parameter of φ_i .
- $c > 0$ is the “global” width parameter.
- The normalization parameter η_i is chosen so that $\langle \varphi_i | \varphi_i \rangle = 1$.

Much depends, of course, on the choice of the $2n + 1$ parameters c , $\{w_i\}$, $\{x_i\}$. For 1-D problems classical mechanics arguments are used in [5] to construct very efficient bases, “tailored” to a given problem. However, such arguments are not readily extended to multi-D, and a simpler approach is applied in [5] in this case. Its rationale can be explained as follows. The highest eigenfunction with energy (approximately) E_{max} is the most oscillatory in low potential regions, while reaching furthest out to high potential regions. Therefore a basis suitable for its approximation will be suitable for all lower eigenfunctions. The most severe oscillations appear near the potential minimum where the local De-Broglie wavelength is $2\pi/\sqrt{2m(E_{max} - V_{min})/\hbar^2}$. Thus the $\{x_i\}$ are chosen in [5] as points

¹A thorough discussion of other types of basis functions is beyond the scope of this work. However, the performance of well chosen Gaussian bases is *good*. In [8] Galerkin b-spline calculations for Morse Hamiltonians are reported. Generally, results obtained there with approximately 100 B-splines have much greater errors compared to results obtained with 48 Gaussians in [5], [7], and in section 4 here (to be fair we note that the Morse Hamiltonians were not identical). Moreover, it is illustrated numerically in the first reference of [8] that eigenvalue errors using n Gaussians scale as α^{-n} while the error using n B-splines of order k scales as $(\frac{1}{n})^{2k}$, *i.e.* the Gaussian error converges asymptotically faster. A thorough analytical and numerical investigation of using high order B-splines in Schrödingers equation is certainly in place. However, we presently opt for Gaussians because of the reasons given above, and because the lessons on node/width distributions we obtain using Gaussians will probably be useful for other types of basis functions including B-splines.

of a regular grid whose spacing is at most $1/4\pi$ of this De-Broglie wavelength (any sufficiently fine spacing would do). On the other hand, the highest eigenfunction is exponentially decaying in the classically forbidden region where $V(x) > E_{max}$, thus the x_i are confined to the classically accessible region $V(x) < E_{max}$. Regular grids are used in [5] which allow an easy notion of grid spacing, however this is by no means a restriction to rectangular grids. For the Henon-Heiles problem the x_i chosen in [5] are points of a regular hexagonal grid pruned to fit within the classically accessible triangular region. Regarding width parameters, the choice $w_i = 1/\Delta x^2$, is advocated in [5]. It is interesting to note that this choice arises if we require the curvature of the φ_i at their centers x_i (i.e. $\frac{d^2\varphi_i}{dx^2}|_{x=x_i}$) to be compatible with the maximal curvature of the highest eigenfunction. Having chosen the w_i we can still vary the global width parameter c . Let us define the matrix S by

$$S_{ij} = \langle \phi_i | \phi_j \rangle . \quad (3)$$

In [5] the most accurate Hamiltonian eigenvalues are obtained for low c values for which the condition number of S is large while still allowing stable numerical calculations.

Hamilton and Light [5] provide efficient Gaussian bases whose centers occupy only relevant regions of configuration space. However, for multi-D problems the density of centers in [5] is constant, and dictated by the highest oscillations in the problem. Such high center density is necessary only in the lowest potential regions. As in the 1-D examples in [5] we expect that sparser Gaussian centers can be taken in higher potential regions. This is the subject of [7], but we first discuss [6] which provides the background for [7], and which unveils important, and surprising, properties of Gaussian bases.

Intuitively, we tend to reject badly conditioned basis functions which are “almost linearly dependent”. Thus we may expect that “good” Gaussian basis functions will not be “too wide” and their centers will not be “too close” together. In [6] Poirier and Light show the contrary; that “good” Gaussian bases can actually have clustered centers and high condition numbers. They regard the choice of Gaussian basis parameters as an optimization problem. Let us define the matrix H by

$$H_{ij} = \langle \varphi_i | \hat{H} | \varphi_j \rangle . \quad (4)$$

Poirier and Light solve for widths and centers which minimize the functional $trace(S^{-1}H)$. This is based on the “variational principle”: each eigenvalue of \hat{H} is smaller than the corresponding eigenvalue of $S^{-1}H$, see MacDonald [9]. Therefore minimizing $trace(S^{-1}H)$ is equivalent to minimizing eigenvalue errors. Note that $S^{-1}H$ represents \hat{H} as a *linear operator* in the non-orthogonal Gaussian basis, while H represents the bilinear form $\langle \cdot | \hat{H} | \cdot \rangle$. Note also that including S^{-1} in our functional we ensure that the Gaussians yielded by the optimization will be linearly independent, however their condition number is not constrained.

An illuminating example is provided by the 1-D harmonic oscillator, $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$. Rather than giving a “well conditioned” basis, the optimization produces Gaussians which are small perturbations of the harmonic oscillator ground state $\psi_0(x) = k_0 e^{-\frac{\alpha^2}{2}x^2}$, where $\alpha = \sqrt{m\omega/\hbar}$. These basis functions have large overlaps, and it is reported in [6] that they reproduce the harmonic oscillator eigenvalues to machine accuracy. At first this may seem surprising, but a simple explanation is provided in [6]. The n 'th harmonic oscillator eigenstate is $\psi_n(x) = k_n e^{-\frac{\alpha^2}{2}x^2} H_n(\alpha x)$, where H_n is the n th Hermite polynomial. Using the formula $e^{-y^2} H_n(y) = (-1)^n \frac{d^n}{dy^n} e^{-y^2}$ (from *e.g.* [10]) we see that $\frac{d^n}{dx^n} e^{-\frac{\alpha^2}{2}x^2} = \left(\frac{-\alpha}{\sqrt{2}}\right)^n e^{-\frac{\alpha^2}{2}x^2} H_n\left(\frac{\alpha}{\sqrt{2}}x\right)$, and therefore ψ_n is in $\text{span}\{\frac{d^k}{dx^k} e^{-\frac{\alpha^2}{2}x^2} | k = 0, \dots, n\}$. Consider now the space mentioned above of Gaussians closely clustered near the potential minimum. It contains difference approximations to the derivatives $\frac{d^k}{dx^k} e^{-\frac{\alpha^2}{2}x^2}$, and since the centers are close together the accuracy of these difference approximations is high. Therefore n closely clustered translations of the ground state span a linear space which gives excellent approximations of the first n harmonic oscillator eigenstates. Clustering of optimal Gaussian centers is observed in [6] also for a Morse potential, however in this case there are several clustering locations away from the potential minimum. The high condition number of such optimal Gaussian bases can be problematic in practical large scale calculations. However, the harmonic oscillator example indicates that high overlaps are needed only to produce accurate approximations of Gaussian derivatives. Poirier and Light therefore propose to include derivatives of Gaussians among our basis functions to begin with, and so avoid the need for large Gaussian overlaps. This direction is not pursued further in [6]. Instead, the bad conditioning of optimal Gaussian bases is addressed by introducing a modified functional,

$$\text{trace}(S^{-1}H) + \lambda \|S - I\| . \quad (5)$$

Gaussians optimizing this functional strike a compromise, depending on the value of λ , between accuracy and conditioning. A similiar functional provides the starting point for [7].

In [7] Garashchuk and Light suggest a practical way of constructing multi-D Gaussian bases, whose node density varies with potential values. They define the functional

$$\text{trace}(H) + \lambda \sum_{i \neq j} \frac{S_{ij}}{1 - S_{ij}} , \quad (6)$$

which is different from the functional (5) used in [6]. Note particularly that $\text{trace}(S^{-1}H)$ from (5) is replaced by $\text{trace}(H)$ in (6). This is minimized for 1-D Morse and double well Hamiltonians to find the density of optimal Gaussian centers $\rho(x_i) = \frac{1}{2(x_{i+1} - x_{i-1})}$ and their widths w_i . It is then observed that $\rho(x_i)$ and w_i fit linear functions of the potential, *i.e.* there are constants a_0, a_1, b_0, b_1 such that $\rho(x_i) \approx a_0(a_1 - V(x_i))$, and $w_i \approx b_0(b_1 - V(x_i))$. A similiar optimization for realistic large

scale problems would be very time consuming. However, Garashchuk and Light regard these two 1-D examples as manifestations of a general rule: “Gaussian bases which have center density and width parameters fitting appropriate linear functions of the potential will be good”. It is also observed in [7] that Hamiltonian eigenvalue errors decrease when the global width parameter c is decreased until unstable numerical calculations set in when $\text{cond}(S) > 10^{12}$. Based on these observations a simple procedure for choosing multi-D Gaussian basis functions is suggested in [7]. Fixing E_{max} and a parameter μ they define the density function

$$\rho(x) = \left(\frac{E_{max} - V(x) + \mu}{E_{max} + \mu} \right)^\gamma. \quad (7)$$

With $\gamma = 1$ the density ρ depends linearly on the potential. The value $\gamma = 1/2$ is also considered in [7], in this case ρ corresponds to the local De-Broglie wave length of the highest eigenfunction. Having defined $\rho(x)$ candidate points x are quasi-randomly generated in the region $V(x) < E_{max}$. x is accepted as a Gaussian center if

$$\rho(x) > r \quad (8)$$

where $r \in [0, 1]$ is random. With the centers at hand, the widths are defined

$$w_i = E_{max} - V(x_i) + \mu > 0. \quad (9)$$

Then c is taken as small as possible until $\text{cond}(S) \approx 10^{12}$.

This approach is applied in [7] to eigenvalue calculations of several multi-D Hamiltonians. The results are much better, or not worse, compared to those of previous methods. Therefore the quasi random distributed Gaussians of [7] appear to be a very good choice. It is our purpose here to make some further observations and suggest a few possible refinements of the approach of [7]. Among other things we shall use the Gaussian basis functions of [7] in a collocation algorithm, which we discuss next.

The collocation approach for finding the eigenvalues and eigenfunctions of a Hamiltonian \hat{H} may be described as follows. First, we choose basis functions $\varphi_1, \dots, \varphi_n$, and a set of points x_1, \dots, x_n called collocation nodes. We then seek functions $\psi = \sum_{i=1}^n u_i \varphi_i$, and eigenvalues E , such that $(\hat{H}\psi)(x_i) = E\psi(x_i)$, $i = 1, \dots, n$. This gives the following generalized matrix eigenproblem

$$\left(-\frac{\hbar^2}{2m} \Delta \Phi + V \Phi \right) u = E \Phi u, \quad (10)$$

where $\Phi_{ij} = \varphi_j(x_i)$, $(\Delta \Phi)_{ij} = \Delta \varphi_j(x_i)$, $V_{ij} = \delta_{ij} V(x_i)$. Since the exact eigenvalues are real we reject solutions with complex E , if there are any. Assuming Φ is invertible (10) is equivalent to

$$\left(-\frac{\hbar^2}{2m} \Phi^{-1} (\Delta \Phi) + \Phi^{-1} V \Phi \right) u = E u \quad (11)$$

and changing coordinates to $y = \Phi u$ we obtain

$$\left(-\frac{\hbar^2}{2m}(\Delta\Phi)\Phi^{-1} + V\right)y = Ey. \quad (12)$$

The matrix on the l.h.s. of (11) is the collocation representation of the Hamiltonian in the φ_i basis, while the matrix on the l.h.s. of (12) is the collocation representation in a basis θ_i , spanning the same function space, and consisting of functions which are 1 on “their” node and zero on all other nodes, $\theta_i(x_j) = \delta_{ij}$.

The collocation approach for spatial discretization of differential operators has a long history [16]. An important mile stone was the introduction of radial basis function (RBF) collocation by Kansa [17], an approach which found much use in the PDEs of classical physics. For recent reviews on radial basis functions and their applications see [19]. RBFs have the form $\varphi_i(x, w_i) = f(\|x - x_i\|, w_i)$, where f is a real valued function peaked at 0 and depending on the parameter vector w , *e.g.* $f(r, w) = e^{-wr^2}$ giving Gaussian RBFs, or $f(r, [w_\alpha, w_\beta]) = (1 + w_\alpha^2 r^2)^{-w_\beta/2}$ giving generalized inverse multi quadric (GIMQ) RBFs (here $w_\beta > d$ where $x \in \mathbb{R}^d$). The centers x_i are usually chosen as the collocation nodes. The attraction of RBF collocation stems from its great flexibility and simplicity. The basis functions shape and location can be adapted to a given problem by carefully choosing parameters. Moreover, the collocation equations are very simple to set up, they do not require calculation of multi dimensional integrals.

The need for efficient methods is particularly acute for high dimensional problems in quantum mechanics. Yang and Peet were the first to show that collocation is feasible for the Schrödinger eigenproblem [13]. They applied collocation to 1-D Morse Hamiltonians together with the Gaussian RBFs of [5], and found that results were as good as the Galerkin approach with the same basis functions. The RBF collocation of [13] has become a standard method for 1-D Schrödinger eigenproblems (appearing as components in more complicated calculations). In multi-D problems collocation did not go, to the best of our knowledge, beyond the stage of initial explorations. Collocation was used for a 2-D problem (Ar-HCl Hamiltonian) in [14] with rectangular grids of nodes and tensor product function spaces. Again, performance was similiar to that of a Galerkin approach with the same basis functions. In [15] collocation was used for the same 2-D problem with Gaussian RBFs whose centers were obtained by truncation of a rectangular grid outside the classically accessible region. However, in [15] only the first three eigenvalues were calculated using an iterative scheme based on projections to low dimensional subspaces. The only example we are aware of for calculation of high (additionally to low) lying eigenvalues and eigenfunctions of multi-D Hamiltonians using RBF collocation is given by Hu, Ho, and Rabitz [11]. The nodes used in [11] were on hexagonal and triangular grids and the basis

functions were the GIMQ RBFs mentioned above. No direct comparison with the Galerkin approach was given in [11].

Having surveyed the topics of Gaussian RBFs and collocation for the Schrödinger eigenproblem we can now venture to take a closer look at some aspects of these topics.

3 Observations and suggestions

Here we give some observations and suggestions which arose while studying the application of Gaussian RBF collocation to Schrödinger equations. Although the term RBFs is used below for Gaussians, some of our observations may be relevant also for other types of RBFs.

1. One of the few methods for constructing efficient function spaces for multi-D quantum problems is given by the quasi random distributed Gaussians of [7]. However, the choice made in [7] for the width parameter of an RBF φ_i depends only on the potential value at *a point*, see equation 9, while φ_i should capture solution properties in *a neighborhood* of x_i . Such properties correspond to the differing nature of the potential function in various regions. Strong repulsions cause molecular potentials to rise very steeply when distance coordinates get small. On the other hand, the smooth interaction of distant particles causes molecular potentials to be much softer for large values of distance coordinates. See for example the Morse potential in figure 1, which is a standard model for two atom molecular potentials.

A possible problem in the width choice of [7] can be illustrated by considering two RBFs φ_i and φ_j such that $V(x_i) = V(x_j)$ are close to the cut off value E_{max} , and such that x_i is in the “hard” region of the Morse potential while x_j is in the “soft” one. Our assumptions imply that φ_i and φ_j will have the same large width. In the soft region this is fine, wide basis functions are compatible with the smooth character of wavefunctions in this region. However a very wide basis function seems unsuitable in the hard region where wavefunction behaviour can change from severe oscillation to rapid decay over a short distance. We therefore conclude that RBFs centered in hard potential regions should generally be narrower than those centered in soft potential regions. This observation is supported by [6] where widths and centers of *optimal* Gaussian RBFs (w.r.t. functional (5)) are found for a Morse potential. Comparing centers with similar potential values we see that the width for a center in the hard region is smaller than for a center in the soft region (see particularly figure 2 in [6]). Recall that functional (5) is different from functional (6) used for optimizing RBF parameters in [7]. While the reasoning giving (5) is

clear, we find no similar justification for (6). Particularly, it is not clear why the representation of \hat{H} as a bilinear form, rather than a linear operator, appears in (6).

We suggest that the parameter choice of [7] may be emiliorated by appropriately decreasing the widths of RBFs, and increasing their density, in hard potential regions. One way to achieve this is to choose nodes and width parameters as in [7] but using a modified potential. Let us denote the classically accessible region by Ω_c , the “soft” potential region by Ω_s , and the “hard” potential region by Ω_h . We define $\tilde{V}(x)$ such that $\tilde{V}(x) = V(x)$ for $x \in \Omega_s \cap \Omega_c$, and such that $\tilde{V}(x)$ has appropriately low values for $x \in \Omega_h \cap \Omega_c$. We may choose, for example, the value of $V(x)$ in a nearby minimum or in the global one. In the classically inaccessible parts of Ω_h we set $\tilde{V}(x) = \infty$, *i.e.* we allow no nodes there. The nodes are then chosen similarly to [7], but using $\tilde{V}(x)$ instead of $V(x)$. Figure 1 illustrates $\tilde{V}(x)$ for a Morse potential. In 1-D and 2-D problems this approach should not pose serious difficulty, the “hard” potential regions and nearby minima may be identified by inspection of the potential surface. In higher dimensions potential surface geometry is not so easy to visualize, yet simple ways may still exist for modifying the choice of nodes and width parameters. We defer their discussion to section 5.

2. In [7], where Gaussian RBFs are used in Galerkin eigenvalue calculations, it is observed that accuracy improves as the global width parameter c is decreased until unstable calculations appear. Therefore $\text{cond}(S)$ is used as an indicator for a good choice of c ; c is chosen so that $\text{cond}(S)$ is in the range $10^9 - 10^{12}$. However, it is desirable that our choice of c will relate to the accuracy of our results in a more direct way, and will give a narrower range of possible c values. We therefore suggest a different approach for choosing c . Let U be a matrix whose columns give (a few or many) approximate eigenfunctions calculated using collocation in the Gaussian RBF basis. Since the exact eigenfunctions are orthonormal we suggest to use the “collocation orthogonalization error” $\|U^*SU - I\|$ as a performance indicator for the choice of c in the collocation approach. To our surprise the values of c minimizing the collocation orthogonalization error were close to those minimizing eigenfunction and eigenvalue errors also in the Galerkin approach. Another criterion for choosing c based on Hamiltonian trace minimization is suggested in section 5.
3. The simplicity of RBF collocation is very appealing. But how does collocation compare to the traditional Galerkin approach? It is reported in [13], [14] that for their basis functions collocation accuracy is similar to that of Galerkin. They therefore conclude that collocation accuracy is similar to that of Galerkin. However, in all our numerical examples the best Galerkin results were better than the best collocation results.

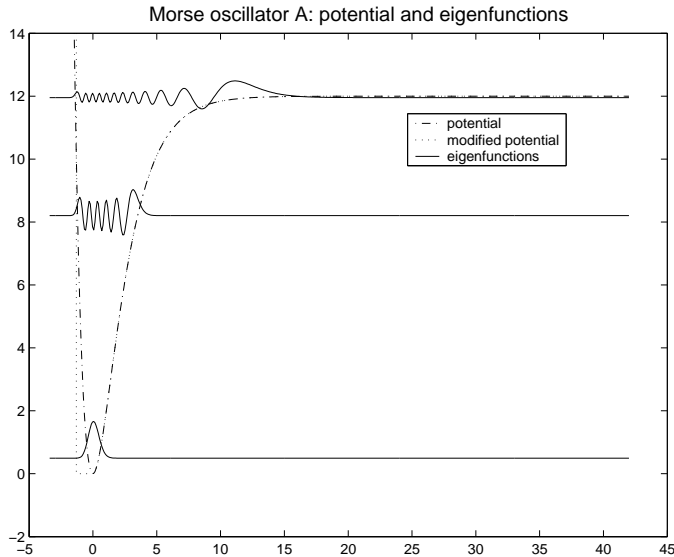


Figure 1: The Morse A potential $V(x) = 12(1 - e^{-0.5x})^2$ is shown here together with the 0th, 10th, and 23rd eigenfunctions. The graph of each eigenfunction is translated vertically by its own eigenvalue. The dotted line is the graph of the corresponding modified potential $\tilde{V}(x)$ defined in equation (13).

Another question is how collocation works together with the quasi randomly distributed Gaussians of [7], *i.e.* how does performance compare to Gaussians whose centers are distributed deterministically with the same density? To the best of our knowledge this was not previously examined in the literature. In our numerical examples collocation performed generally worse with the quasi random centers.

4 Numerical examples and discussion

The suggestions and observations above were tested on two Hamiltonians which we call Morse A, and Morse B. Morse A, from [13], has potential $V(x) = 12(1 - e^{-0.5x})^2$ which is plotted in figure 1, and parameters $m = 6$, $\hbar = 1$. This system has 24 bound states. Morse B has the potential $V(x) = 12(1 - e^{-0.9566x})^2$, and all other parameter values identical to those of Morse A. This system has 13 bound states. Analytic formulas for eigenvalues and eigenfunctions were taken from [18].

For each Hamiltonian three sets of Gaussian basis functions were tested. All consisted of 48 Gaussians, the parameter values $E_{max} = 12$, $\mu = 0.02$ were used in the construction of all, and all had nodes in an interval $[L, R]$. L is the left classical turning point for $E_{max} = 12$ with values $L \approx -1.3863$,

and $L \approx -0.7246$, for system A and B respectively. R was chosen arbitrarily (with a few trials), but well within the region where the highest bound state has decayed close to zero. The values $R = 40$, and $R = 50$, were chosen for system A and B respectively (in both cases the right classical turning point for $E_{max} = 12$ is too big for our purposes). The method for choosing nodes and width parameters in each set of basis functions follows.

1. Set 1: Nodes were generated so: $x_1 = R$, $x_{i+1} = x_i - k/\sqrt{E_{max} + \mu - V(x_i)}$, where k was chosen so that $x_{48} = L$. This corresponds to the node density of [7] with $\gamma = 1/2$, see equation (7). Having the nodes, the width parameters were chosen as specified in equation (9).
2. Set 2: The nodes were generated quasi randomly as specified in [7] with the same density as in basis 1. The Sobol sequence software package by W. Putschögl [12] was used. Having the nodes, the width parameters were chosen as in basis 1.
3. Set 3: We regard the left half line $x < 0$ as the hard potential region for both our Morse potentials. Accordingly, set 3 was generated as set 1, but using the following modified potential function, which is illustrated in figure 1,

$$\tilde{V}(x) = \begin{cases} V(x) & x > 0 \\ 0 & L \leq x \leq 0 \end{cases} . \quad (13)$$

The nodes and width parameters of sets 1A, 2A, 3A, are illustrated in figure 2 (this obvious notation distinguishes between basis sets for Hamiltonians A and B). The nodes of set 3A are illustrated in figure 3 together with the 23rd eigenfunction, the compatibility between node density and eigenfunction oscillation is evident. The node density given by equation (7) with $\gamma = 1$ was also tested, but results were better with $\gamma = 1/2$ as above.

For each basis set the Hamiltonian was discretized using collocation with the x_i serving as collocation nodes, and using Galerkin with analytic calculation of matrix elements. The average eigenvalue error

$$\epsilon_v = \frac{1}{N+1} \sum_{n=0}^N |E_n^a - E_n| , \quad (14)$$

and the average L_2 norm of eigenfunction errors

$$\epsilon_f = \frac{1}{N+1} \sum_{n=0}^N \|\psi_n^a - \psi_n\|_{L_2} , \quad (15)$$

were calculated for different values of the global width parameter c . The superscript a stands for “approximate”, and $N = 23$ or 12 for system A or B respectively. Results are shown in figures 4, 6.

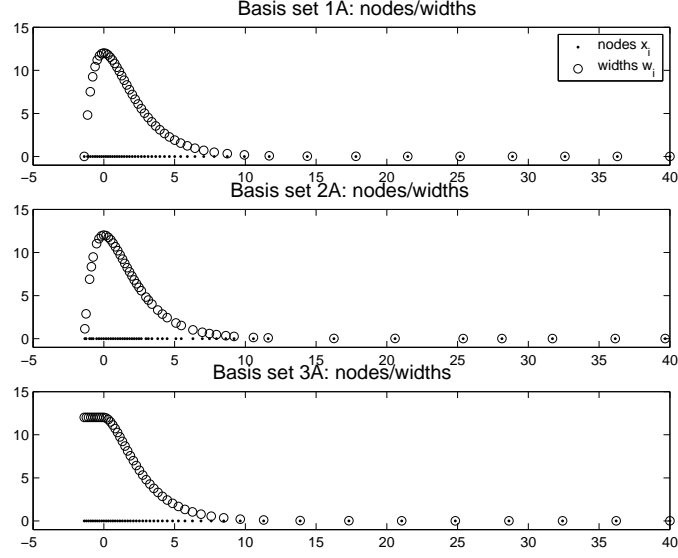


Figure 2: Nodes x_i (dots: \cdot) and width parameters w_i (circles: \circ) used for the different kinds of basis functions. Set 1A: deterministic node choice. Set 2A: quasi random node choice [7]. Set 3A: deterministic node choice with density corresponding to the modified potential in equation (13). See section 4 for a full explanation of these parameter choices.

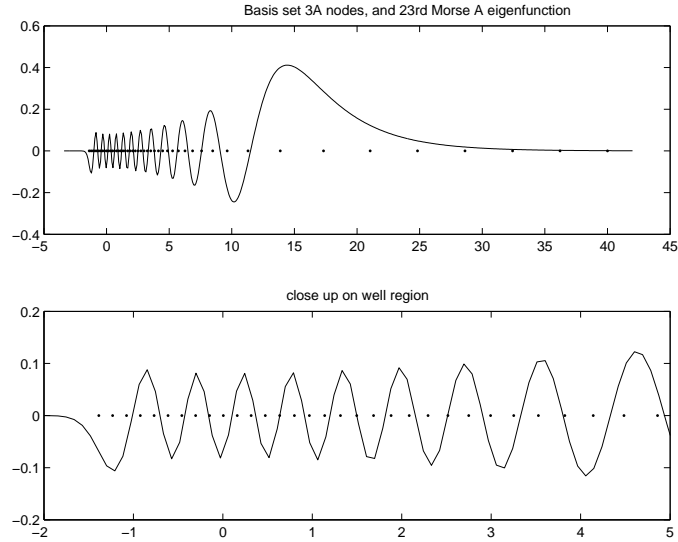


Figure 3: Nodes of basis set 3A and 23rd Morse A eigenfunction. Note the compatibility between eigenfunction oscillation and node density. The bottom graph shows a close up on the well region.

These figures also illustrate the c dependence of the collocation orthogonalization error

$$\|U^*SU - I\|_{Frobenius} , \quad (16)$$

with U being the $48 \times (N + 1)$ matrix of eigenvectors calculated by collocation. Table 1 gives $cond(S)$ and $cond(\Phi)$ at the c values minimizing ϵ_f for each basis set and discretization method. The only exception is in basis 2B where the minimizing c values gave very ill conditioned bases. Instead larger c was taken so that $cond(S) \approx 10^{12}$ as advocated in [7]. For the different discretization methods and bases (with the c values of table 1) the logarithms of eigenvalue and eigenfunction errors are plotted against their index in figures 5, 7, 8, 9.

Figures 8 and 9 show that basis sets 3 gave orders of magnitude better results compared to basis sets 1 and 2, except for a few high eigenfunctions/eigenvalues where accuracy was similar. This indicates that indeed there is room for improvement in the method of [7] for choosing nodes/widths in hard potential regions. Moreover, the modification suggested here in basis set 3 can produce highly accurate results.

The results for basis sets 1 and 3 in figures 4, 6, (top and bottom rows) indicate that it may be possible to choose the global width parameter c based on the collocation orthogonalization error. The minimum of ϵ_f for collocation, and for Galerkin, occurs near minima of the collocation “orth err”. In some cases these minima occur for c values for which $cond(S)$ is not too large, see table 1. This supports our notion that it is desirable to have a criterion for choosing c which is more refined than reaching large $cond(S)$. Similar relations between minima of ϵ_f and of the collocation orthogonalization error were not observed in basis sets 2 with the quasi randomly distributed nodes [7].

The simplicity of collocation is an important advantage which can save much programing time. Moreover, with a careful choice of basis function parameters collocation can give accurate results. However, figures 5, 7 illustrate that in all our calculations the Galerkin results were much more accurate than those of collocation.

Examining the bottom row in figures 8, 9, we see that collocation errors were larger with bases 2A and 2B compared to bases 1A and 2A. That is, we see that larger errors appeared when using collocation with quasi random DGBs, compared to DGBs whose centers had the same density but were chosen deterministically.

5 Conclusions and future directions

In this work several observations about Gaussian radial basis functions and collocation in Schrödinger eigenproblems were made and tested numerically. It may be hoped that the following conclusions are relevant not only for choosing good Gaussian bases, but also for other types of localized radial basis functions.

In [7] Garashchuk and Light give one of the few examples of efficient basis functions for multi-D Schrödinger equations. An improvement of their approach may be obtained from our observation that the Gaussians of [7] are too wide in “hard” potential regions, *e.g.* where nuclei are close together in molecular potentials. This led us to suggest choosing nodes/weights using the method of [7], but with a modified potential function obtained by replacing steeply rising parts by “vertical” walls and flattening nearby valley regions. We emphasize that our goal is to produce basis functions which are not overly wide and sparse in hard potential regions. Using the modified potential above is just one way to achieve this goal, others are suggested in the future directions below. Our numerical tests indicate that the changes we propose in the choice of nodes/widths can give a dramatic improvement in accuracy.

In the literature we often encounter the conception that with appropriately wide basis functions collocation errors are not larger than those of Galerkin [13], [14], [15]. However, in our numerical tests the Galerkin accuracy was better than that of collocation, often orders of magnitude better. The difference is probably because we have chosen the optimal global width parameter for each method, while in [13], [14], [15] no special attempt was made to optimize c . Our calculations indicate that caution should be exercised before embracing collocation as equally accurate to Galerkin.

In [7], [13], and other places, it is suggested to decrease the global width parameter, making basis functions wider, until the basis is nearly badly conditioned. However a more refined method for choosing c is desirable. One supporting fact is that the optimal c values in table 1 indeed give large $cond(S)$ but not quite as large as expected in the literature. Our numerical tests indicate that the collocation orthogonalization error, defined in equation (16), may guide us in choosing the global width parameter. We found that minima of the collocation orthogonalization error plotted against the global width parameter occur near minima of eigenfunction/eigenvalue errors calculated by collocation and by the Galerkin approach.

For the future, it may be profitable to attempt a further refinement of the choice of nodes/widths in “hard” potential regions. Suppose we have nodes/widths constructed by some distribution method, *e.g.* that of [7]. Methods should be explored for identifying nodes lying in hard potential regions,

for adding more nodes to these regions, and for choosing width parameters with respect to potential values in a neighborhood and not just a point. It seems feasible that these goals can be achieved for high dimensional systems using only simple local calculations.

Apart from choosing the centers and relative widths of radial basis functions, a correct scaling of their widths through the global width parameter c is critical for good performance. Our suggestion of using the collocation orthogonalization error as a criterion for choosing c may be worth pursuing. One possibility is to avoid full diagonalization of the collocation Hamiltonian matrix and to measure the orthogonalization error only for the few lowest, or highest, eigenvectors. An even simpler method may be tried in the Galerkin approach where the “variational principle” holds. In this case the trace of the Hamiltonian matrix is minimal for the optimal c (w.r.t. eigenvalue errors). A very simple method for choosing a “good” c may possibly be based on this observation. The work required will not be larger compared to the method used in [7] based on the condition number of S^{-1} . Some modifications may also be examined. For example, if the matrix elements of H are not calculated exactly we may try to choose c by minimizing the first few eigenvalues of $S^{-1}H$.

Recall from section 3 that optimization of functional (5) gives nodes/widths which are consistent with our observations. So it may be interesting (but probably difficult) to apply the ideas of Garashchuk and Light from [7] but with the functional (5), rather than the functional (6). That is, to attempt identifying a functional form for the densities and width parameters arising from optimization of functional (5).

Finally, in addition to further numerical work, a mathematical error analysis for RBFs applied to Schrödingers equation should be attempted.

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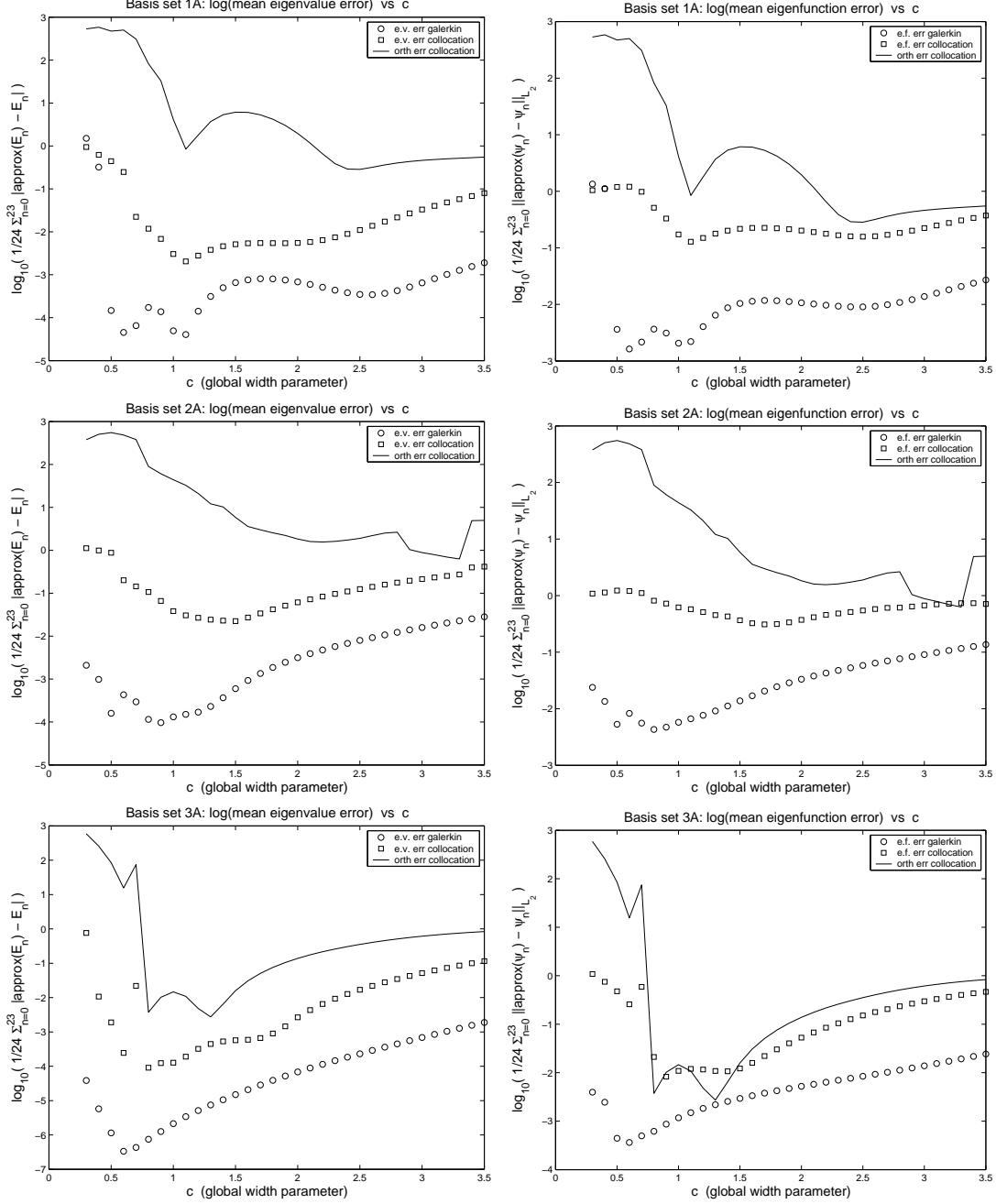


Figure 4: Error dependence on global width parameter, Morse A: Logarithms of mean eigenvalue (left column) and eigenfunction (right column) errors plotted against the global width parameter for the different basis sets (rows), and discretization methods, applied to Morse Hamiltonian A. Circles-Galerkin, squares-collocation, continuous line-“orth error” which is defined in equation (16). See table 1 A for information on the condition numbers of S and Φ .

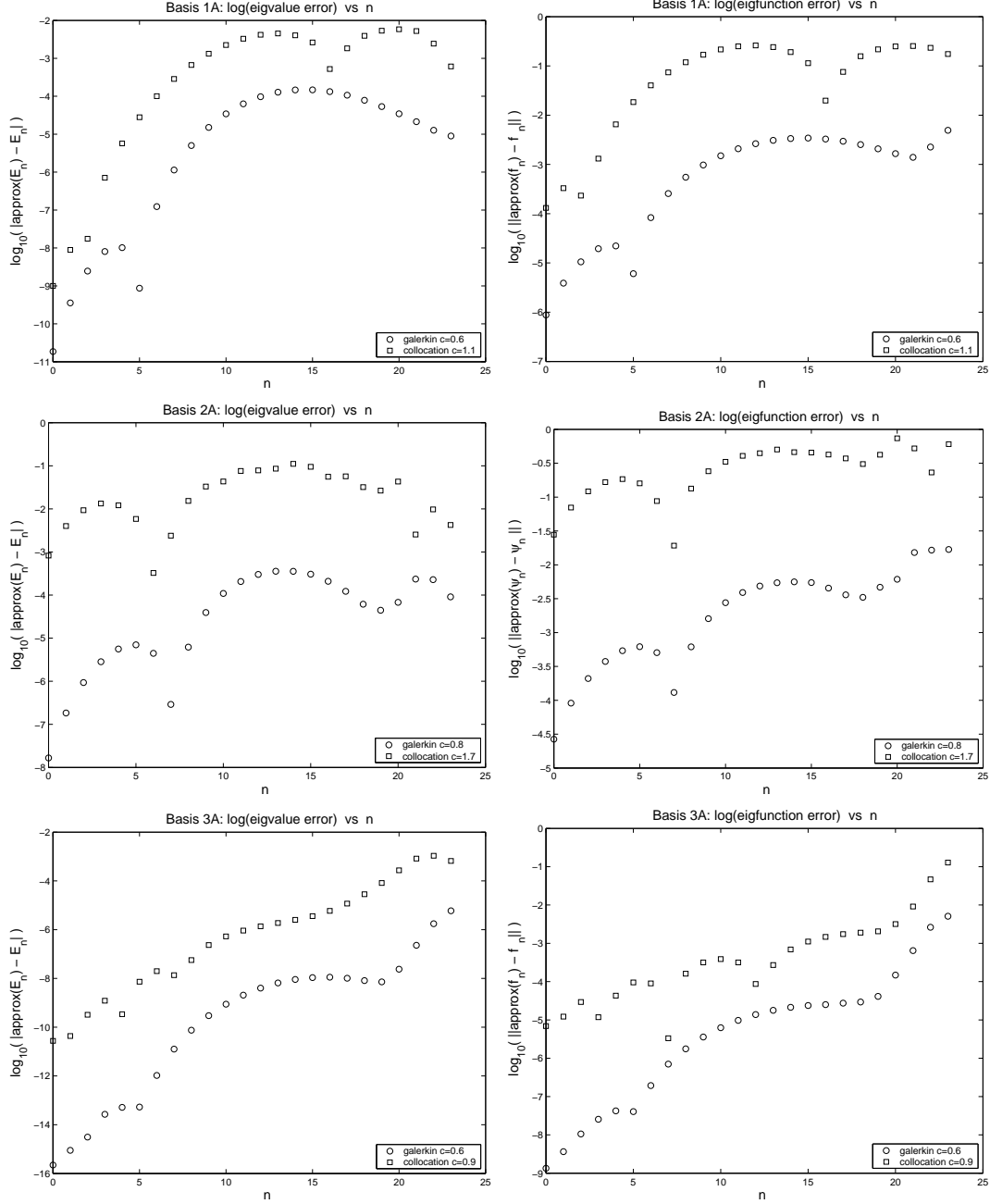


Figure 5: Comparing collocation and Galerkin performance, Morse A: Logarithms of eigenvalue (left column) and eigenfunction (right column) errors vs. index for each basis set (rows) and each discretization method (Circles-Galerkin, squares-collocation) applied to Morse Hamiltonian A. In each case results were obtained using the global width parameter value which minimizes the mean eigenfunction error ϵ_f , see table 1 A. Note the low errors in the Galerkin/basis set 3 combination.

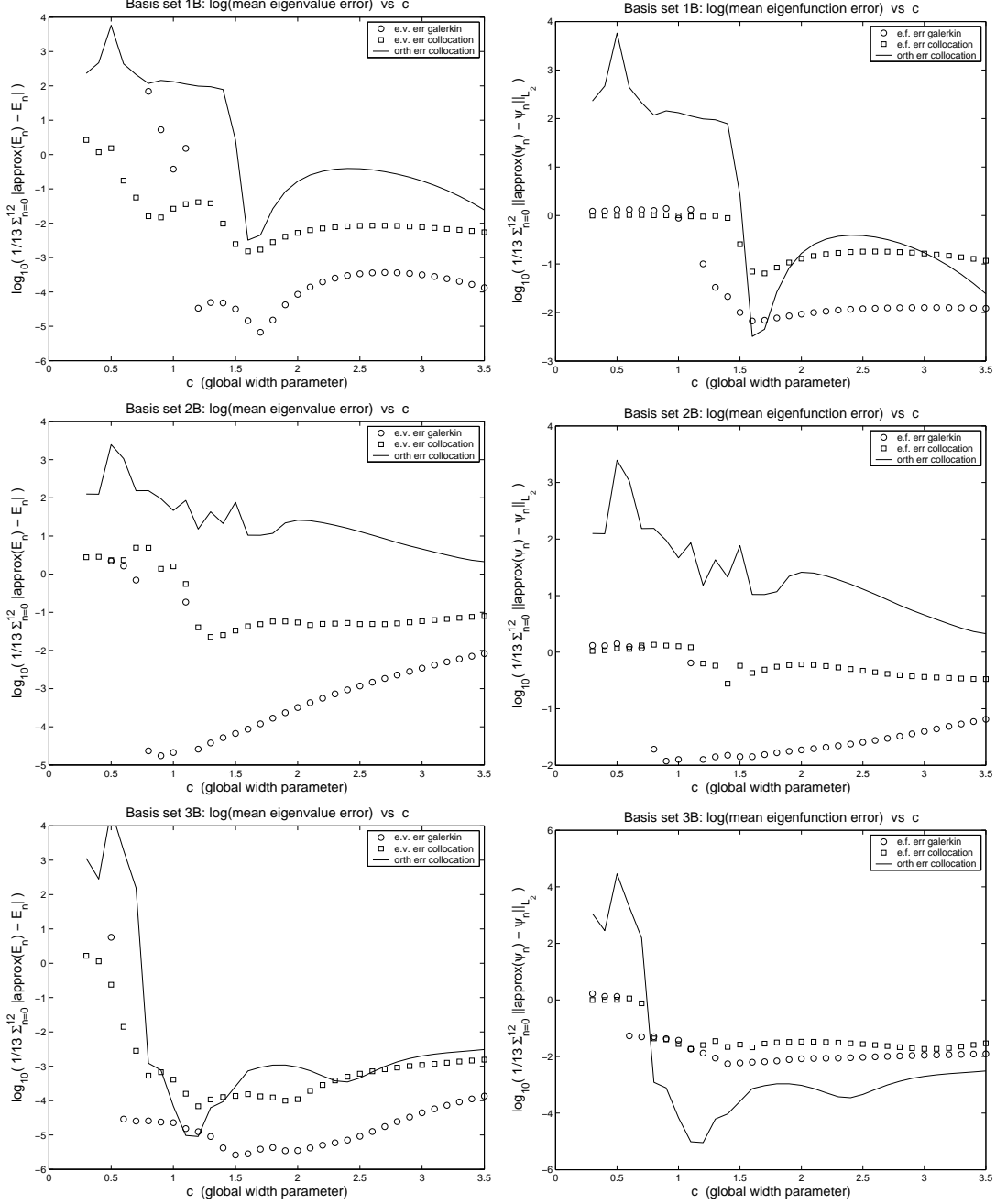


Figure 6: Error dependence on global width parameter, Morse B: Logarithms of mean eigenvalue (left column) and eigenfunction (right column) errors plotted against the global width parameter for the different basis sets (rows), and discretization methods, applied to Morse Hamiltonian B. Circles-Galerkin, squares-collocation, continuous line-“orth error” which is defined in equation (16). See table 1 B for information on the condition numbers of S and Φ .

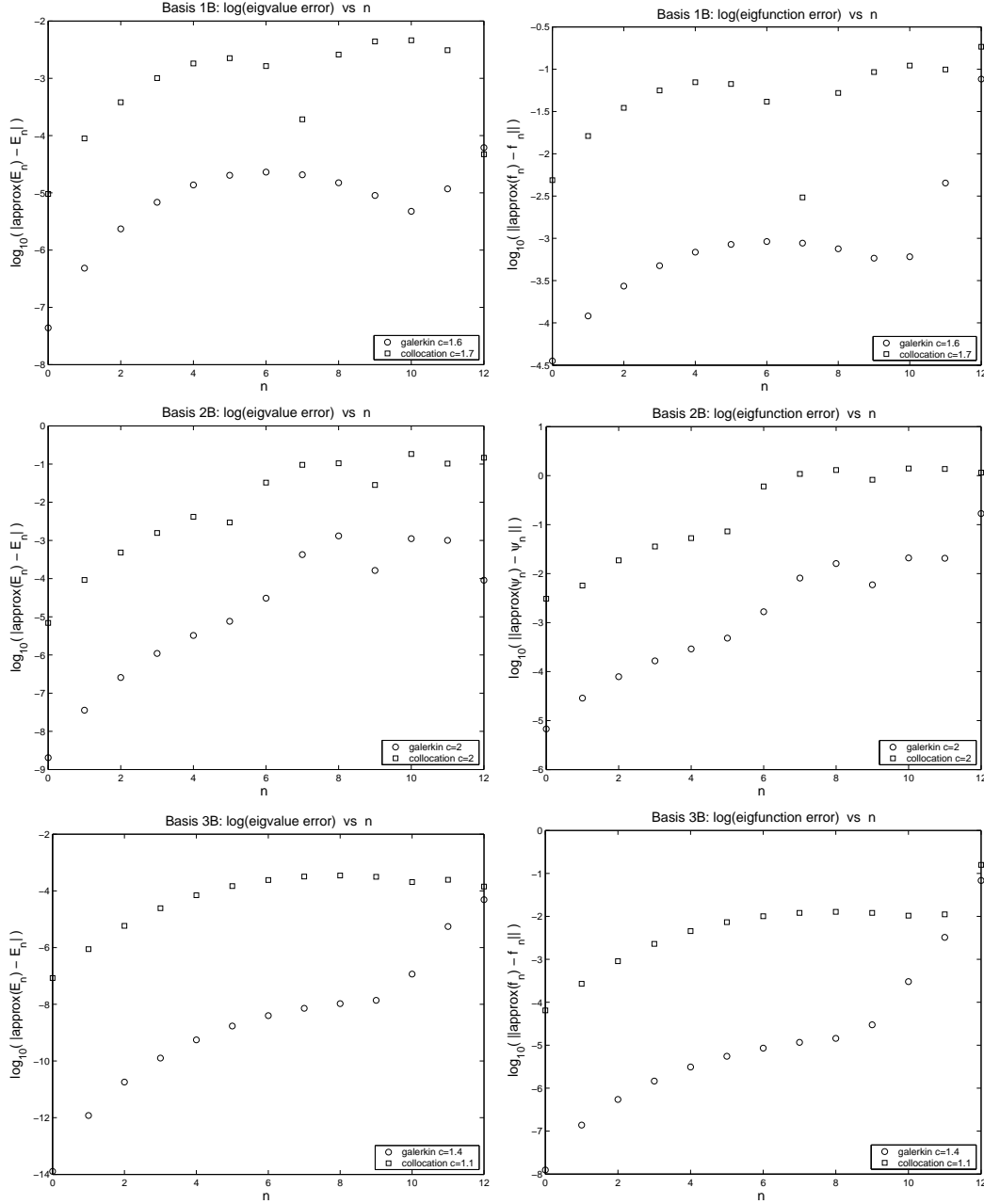


Figure 7: Comparing collocation and Galerkin performance, Morse B: Logarithms of eigenvalue (left column) and eigenfunction (right column) errors vs. index for each basis set (rows) and each discretization method (Circles-Galerkin, squares-collocation) applied to Morse Hamiltonian B. In each case (with the exception of basis 2B) results were obtained using the global width parameter value which minimizes the mean eigenfunction error ϵ_f , see table 1 B. Note the low errors in the Galerkin/basis set 3 combination.

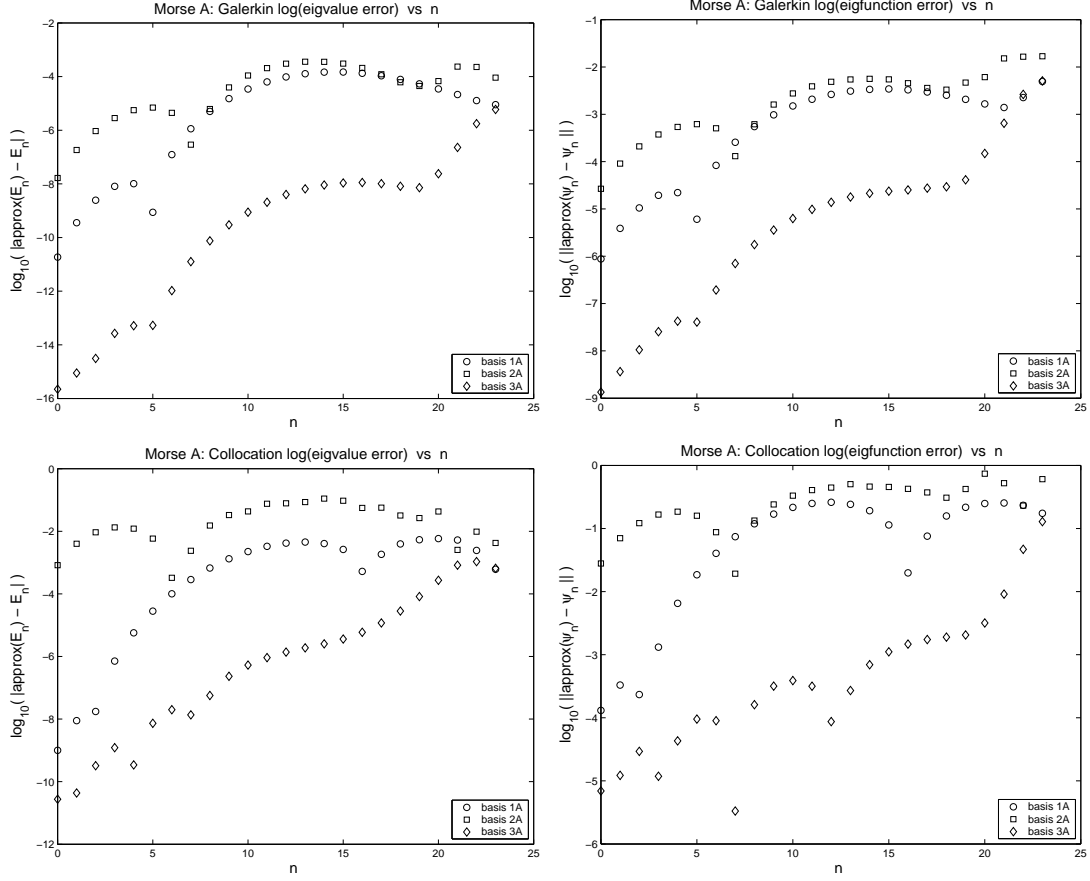


Figure 8: Comparing the different basis sets, Morse A: Logarithms of eigenvalue (left column) and eigenfunction (right column) errors vs. index for each discretization method (rows) and each basis set (circles-set 1A, squares-set 2A, diamonds-set 3A) applied to Morse Hamiltonian A. In each case results were obtained using the global width parameter value which minimizes the mean eigenfunction error ϵ_f , see table 1 A.

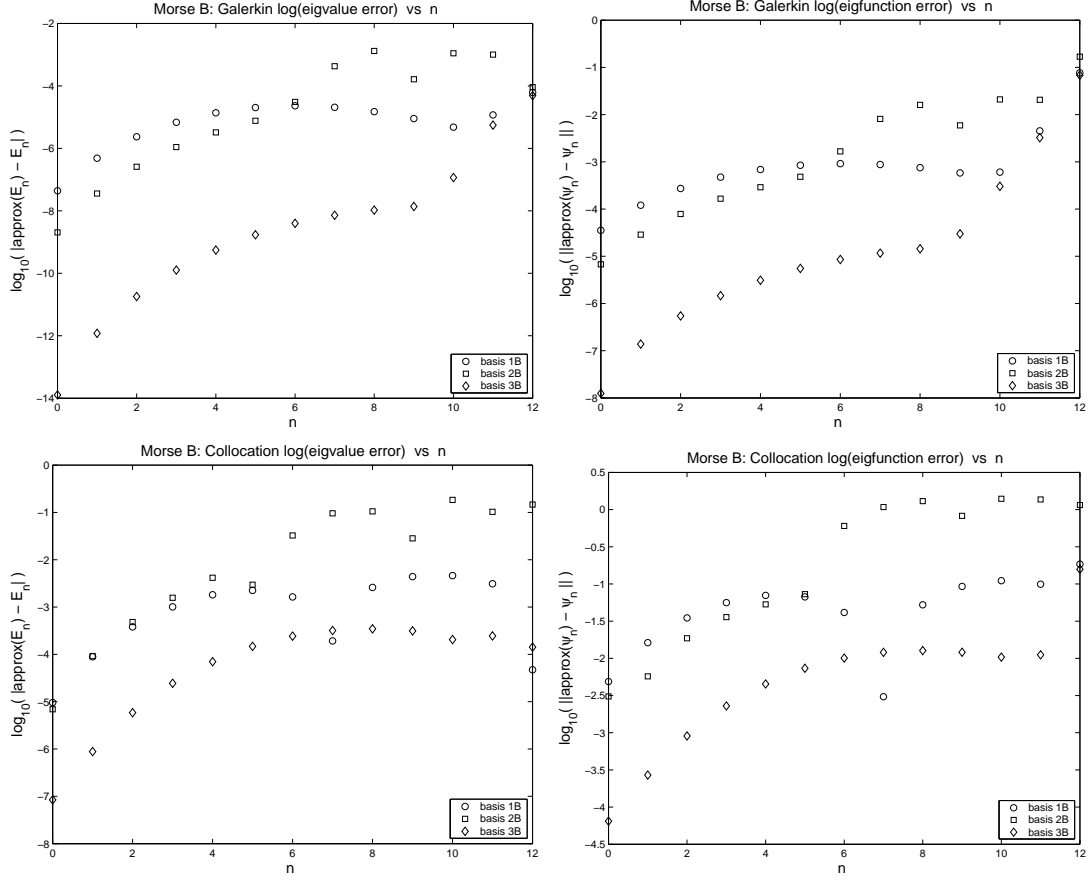


Figure 9: Comparing the different basis sets, Morse B: Logarithms of eigenvalue (left column) and eigenfunction (right column) errors vs. index for each discretization method (rows) and each basis set (circles-set 1B, squares-set 2B, diamonds-set 3B) applied to Morse Hamiltonian B. In each case (with the exception of basis 2B) results were obtained using the global width parameter value which minimizes the mean eigenfunction error ϵ_f , see table 1 B.

	basis set 1A		basis set 2A		basis set 3A	
	Galerkin	collocation	Galerkin	collocation	Galerkin	collocation
c	0.6	1.1	0.8	1.7	0.6	0.9
$cond(\Phi)$	4.07×10^{10}	3.99×10^3	6.73×10^6	480	1.2×10^8	6.53×10^4
$cond(S)$	4.4×10^9	8.9×10^4	6.97×10^8	7.3×10^4	4.76×10^9	9.66×10^6

	basis set 1B		basis set 2B		basis set 3B	
	Galerkin	collocation	Galerkin	collocation	Galerkin	collocation
c	1.6	1.7	2	2	1.4	1.1
$cond(\Phi)$	4.12×10^7	6.71×10^6	1.46×10^9	1.46×10^9	5.31×10^7	1.02×10^8
$cond(S)$	3.98×10^8	2.21×10^8	1.85×10^{12}	1.85×10^{12}	4.28×10^9	1.96×10^{10}

Table 1: The condition numbers of Φ and S are given at the c (global width parameter) values minimizing the mean eigenfunction error ϵ_f (defined in equation (15)) for each basis set and each discretization method applied to systems A and B. For basis 2B the non optimal value $c = 2$ was chosen since the associated $cond(S)$ has the maximal value advocated in [7]. The optimal values were $c = 0.9$ for Galerkin, with $cond(S) = 1.68 \times 10^{17}$, and $c = 1.4$ for collocation, with $cond(S) = 7.79 \times 10^{14}$.

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